R&D Plans for Przm/Exams (AgDrift/Bass)

Task Plan 6519b: Conduct Probabilistic Exposure and Ecological Risk Assessment of Pesticides via Simulation Modeling

Lawrence A. Burns, Ph.D.

Task 6519b (*APRAT*) Peer Review

December 7, 2000

GPRA Goal 4 Staffing & Budget

- 1 FTE - Lawrence A. Burns, $0K R&D
- with (unpaid) cooperation and assistance:
  - OPP ECOFRAM Implementation Team
  - Robert Ambrose (bbl transport, sediment)
  - Craig Barber (BASS)
  - Sandra Bird (AgDrift)
  - Robert Carousel (PRZM)
  - Lourdes Prieto (GIS support)
  - Luis Suárez (database development software)

Regulatory Modeling
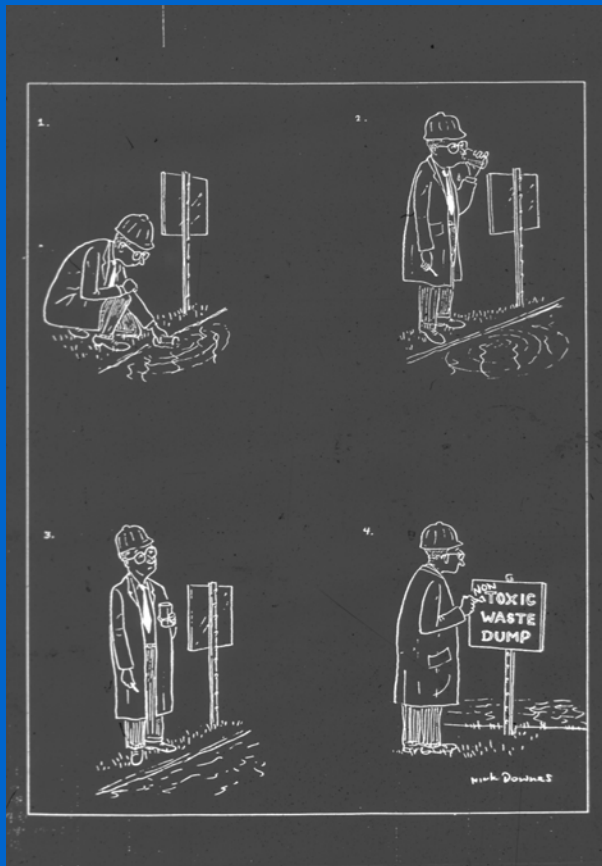
- Replace expert opinion with a "consistent, predictable, trans-parent" regulatory process
- Extend new chemical data to field conditions: Models
- Tier 1: GENEEC
- Tier 2:
  - AgDrift - aerial spray
  - PRZM - in the field
  - EXAMS - in the water
  - BASS - fishes

Themes and Objectives

- Support of "Tier 2" exposure analysis
  - Maintain AgDrift/PRZM/EXAMS as the core of Agency exposure assessment modeling
  - Models both "stand-alone" and file-linked
- Database Modernization
  - NRI agricultural crop/soil
  - SAMSON/HUSWO meteorology (35 year)
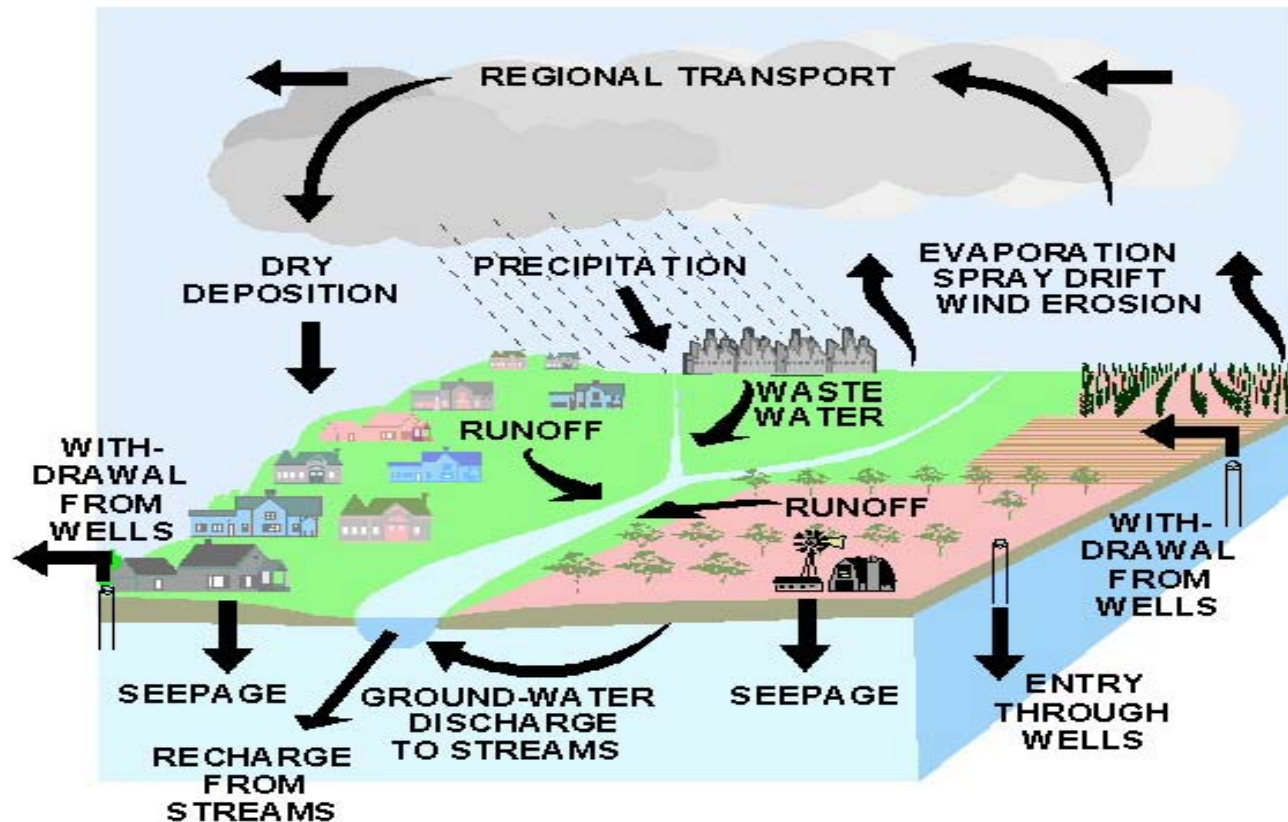- Migrating towards Tier 2 probabilistic, nation-wide assessments (ECOFRAM)

Themes and Objectives

- Science Modernization
  - Green-Ampt infiltration, Penman-Monteith ET_0
  - Sorption kinetics, bbl transport
  - New documentation and test of solar spectral irradiance code (photolysis, singlet oxygen)
- Technology Modernization
  - Modernize PRZM code (Fortran 95)
  - GUIs, link SubPart N/OECD data requirements
  - Output graphics in probabilistic framework
  - Link model parameters to GIS data (MIMS)

Conceptual Models

- Conservation of mass and full pathway accounting are the organizing principles

- Regional scale sets the framework

- Small watershed at the farm scale sets the PRZM/EXAMS "scenario"

- Ecosystem scale defines the pathways, processes and phenomena for modeling
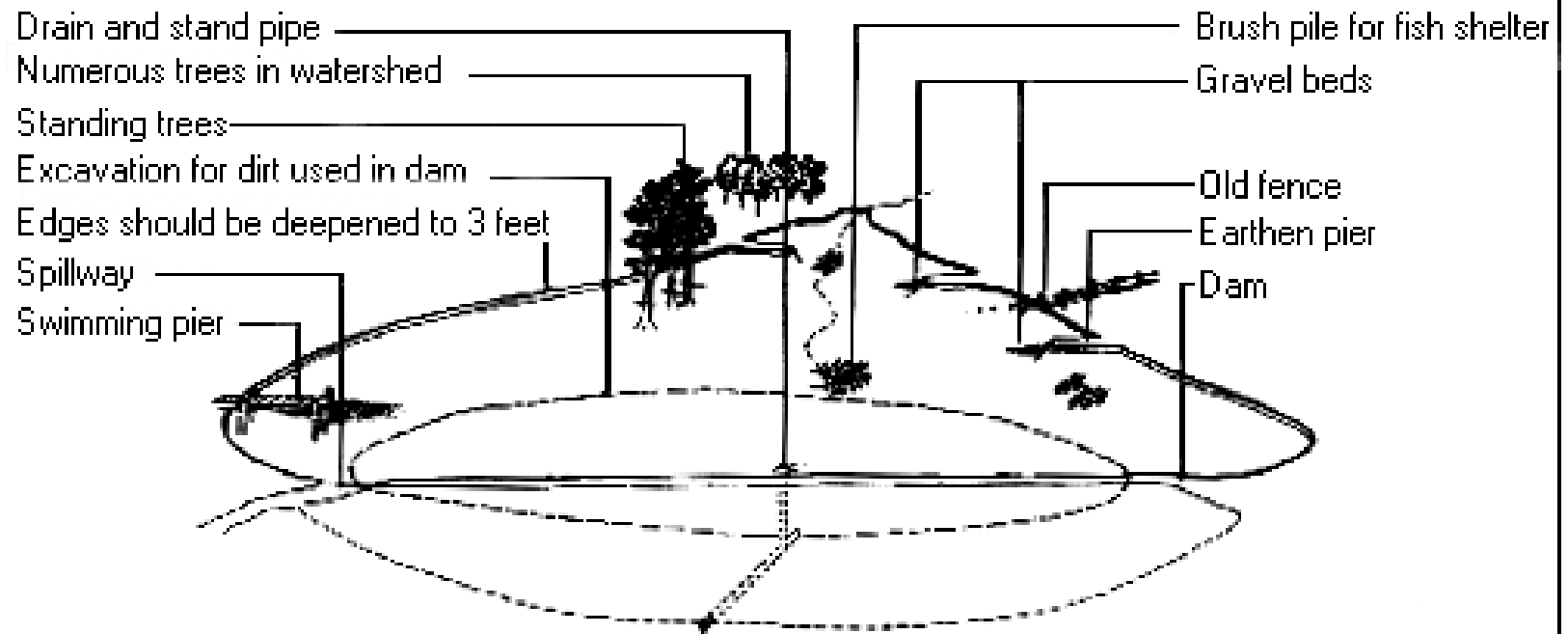
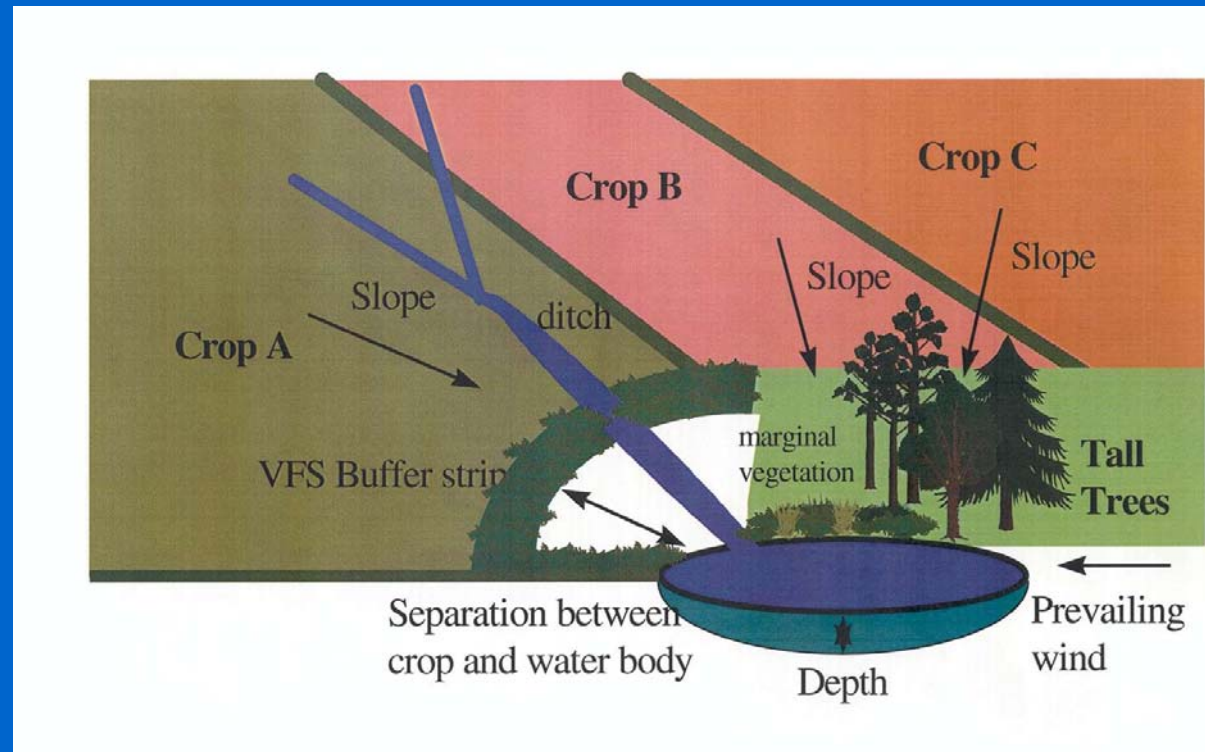# Regional Scale Concept

Farm Scale Watershed

Farm Pond Design

Drain and stand pipe — Brush pile for fish shelter
Numerous trees in watershed — Gravel beds
Standing trees —
Excavation for dirt used in dam — Old fence
Edges should be deepened to 3 feet — Earthen pier
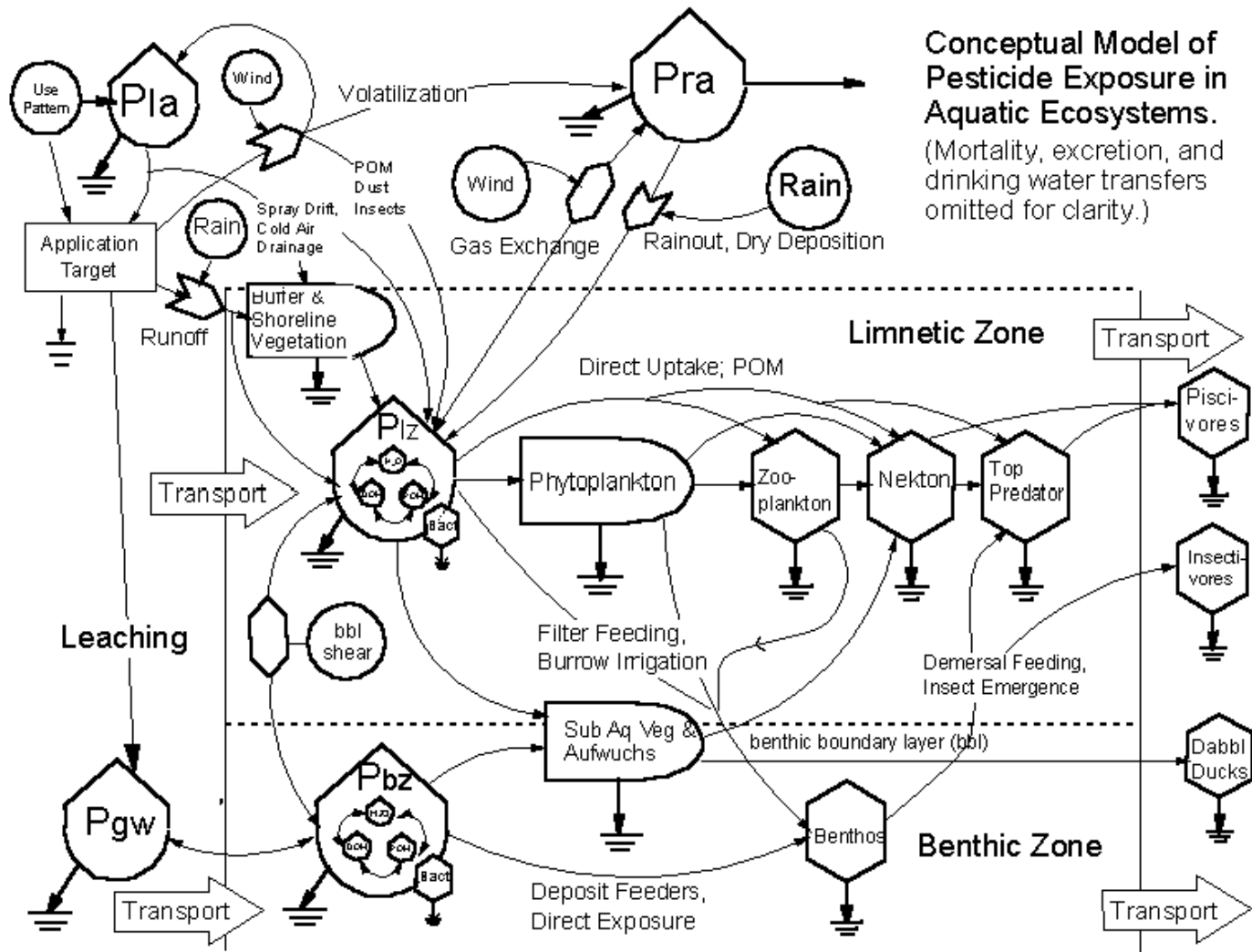Spillway — Dam
Swimming pier —

Model Watershed Scenarios

- Multiple crops
- Multiple soils
- Surface drains
- Tile drains
- Drift barriers
- MLRA pond geometries and drainage areas

Formal Ecosystem Model

Conceptual Model of Pesticide Exposure in Aquatic Ecosystems.
(Mortality, excretion, and drinking water transfers omitted for clarity.)

Off Site Drift of Pesticides

Sandra L. Bird

Primary Drift ⟺ Secondary Drift

- Minutes to hours
- Near to medium range
- Independent of properties of active ingredient
- Application equipment controls
- Local meteorology at application is primary environmental driver

- Hours to weeks
- Near to long range
- Dependent on chemistry of active ingredient
- Independent of application equipment
- Many environmental factors affect drift

AgDrift Current Version

General ⟷ Structure

General
- Primary drift only
- Near-field focus
- Developed for program office applications
- Developed in CRADA
- Developed as an ecological assessment tool
- Applicable to human exposure issues

Structure
- 3 tiers (screening, label mitigation, site specific)
- Mechanistic aerial application
- Empirical ground and orchard sprayer
- Windows interface
- Libraries (aircraft, meteor-ology, drop size distribution,)
- Assessment utilities toolbox
- On-line help

AgDrift Enhancements

- Mechanistic ground spray model

- Medium range drift model

- Seamless linkage to PRZM/EXAMS and ecological exposure modeling

- Improved nozzle modeling

New, Longer-Term Enhancements

- Mechanistic orchard model

- Drift mitigation factors

- Human exposure tools; integration into human health modeling framework

- Linked primary and secondary drift modeling

the Pesticide Root Zone Model
Robert Carousel

- Hydrology - runoff, erosion, infiltration
- Chemical transport
  - multiple pesticides
  - metabolites
- Volatilization
- Crop plants
  - foliar gas exchange
 - uptake from soil solution

PRZM

Pesticide Root Zone Model

PRZM simulates the runoff and the vertical movement of pesticides in the unsaturated soil, within and below the plant root zone. The model consists of hydrology and chemical transport components that simulate runoff, erosion, plant uptake, leaching, decay, and foliar washoff of a pesticide.
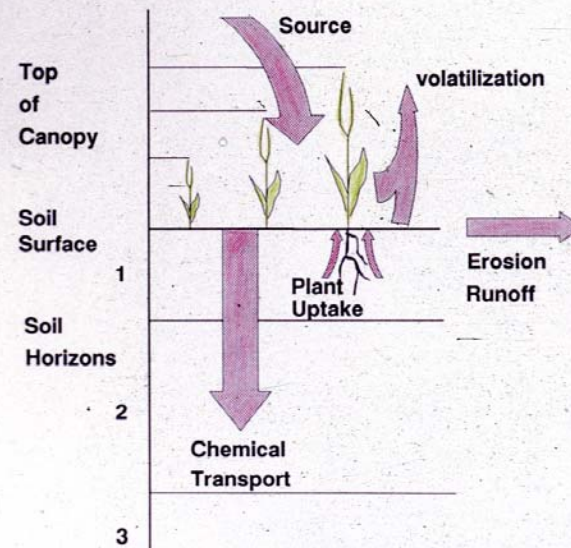
PRZM Input Data Management

- Crop phenology
  - planting dates, ...
- Meteorology-Samson
- Agronomic practices
- Soil properties
- Pesticide use pattern
  - application rate, …
- Chemical properties
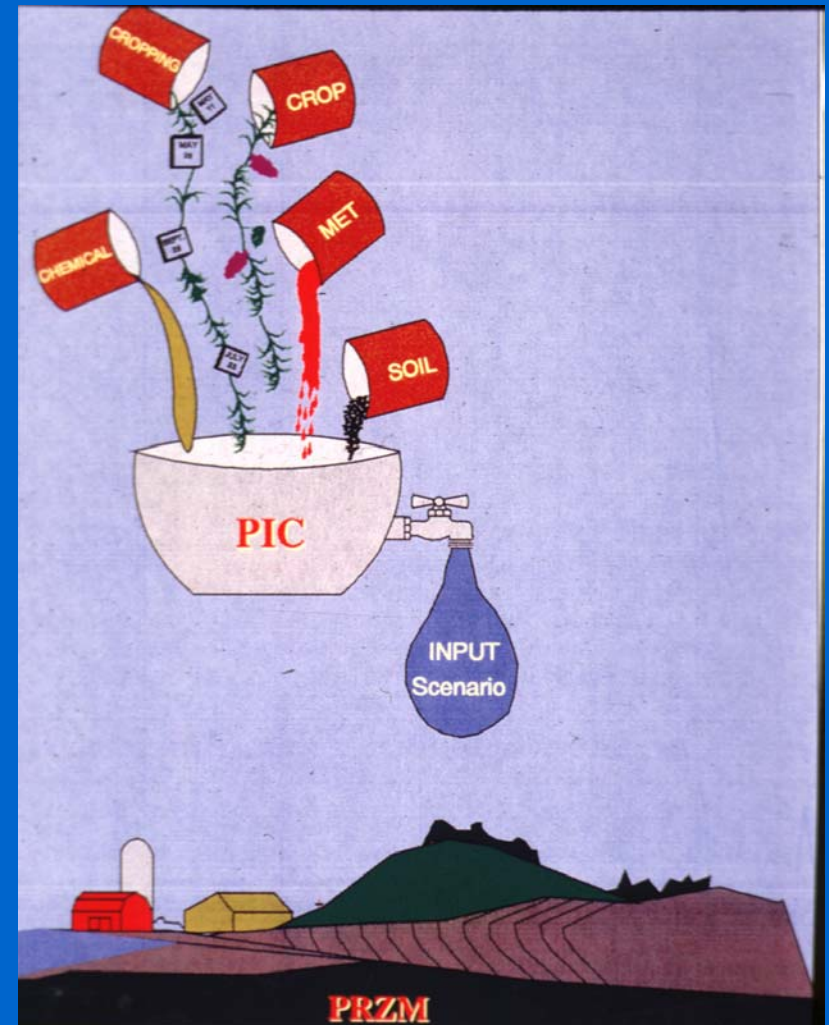
Improvements to PRZM Hydrology

- Unchanged Since 1982
- Two key empirical infiltration parameters
  - USDA Curve Number Technique (CN)
  - Water movement based on field capacity (FC)
- Combine four newer infiltration science advances:
  - Chu infiltration model
  - Clapp wetting front model
  - Clapp and Hornberger soil water retention model
  - Miller scaling theory

PRZM Hydrology Modifications

- Chu Infiltration Model
  - Modified Green/Ampt
  - Uses hydraulic conductivity (K) of the wetted zone, the wetting front suction (ψ), and the difference in the average soil water content before and after infiltration.
  - Physical parameters
    - Available from USDA databases
    - Can be directly measured in the field
    - Estimated from Clapp and Hornberger Soil Water Retention Model

PRZM Hydrology Modifications

- Clapp Wetting Front Model
  - Subsurface distribution of soil moisture calculated from soil physics and basic hydraulic properties of soils
  - Soil profile is portrayed as a series of "blocks", each having a depth and a uniform soil-water content.
  - Fluxes at individual moisture blocks are computed, and these flux values are used to move the wetting fronts upward or downward.
  - The widths of the blocks change, representing a change in the average water content in response to the fluxes.

PRZM Hydrology Modifications

- Clapp and Hornberger Soil Water Retention Model
  - Soil water retention curve relating tension or suction ψ to volumetric water content θ.
- Miller Scaling Theory: taking

$$K_S, \theta_S \ = \text{Reference values}$$

$$K_S{}^*, \theta_S{}^* = \text{Scale adjusted values}$$

$$S_s = \text{Scale factor}$$

PRZM Hydrology Modifications

- Using scaling theory
  - Standard deviation $\sigma(S_S)$ is used to derive a sequence of S_s values, each having its associated probability. These S_s are used to calculate a suite of K_S^*, θ_S^* values from the reference values K_S, θ_S
  - Scale factor taken as log-normally distributed
  - the Clapp Wetting Front (sub-)model then simulates the water balance and computes water outputs for each realization of the soil-water parameters

# Exposure Analysis Modeling System
Lawrence Burns

- Loadings from PRZM and AgDrift

- Combines pesticide chemistry with aquatic ecology/limnology

- Parent and metabolites

- Limnetic and benthic exposure simulated

- Data transfer to BASS

- 3MRA/TRACE(Wasp) core technology

Schematic Diagram of Important Processes in Environmental Photochemistry
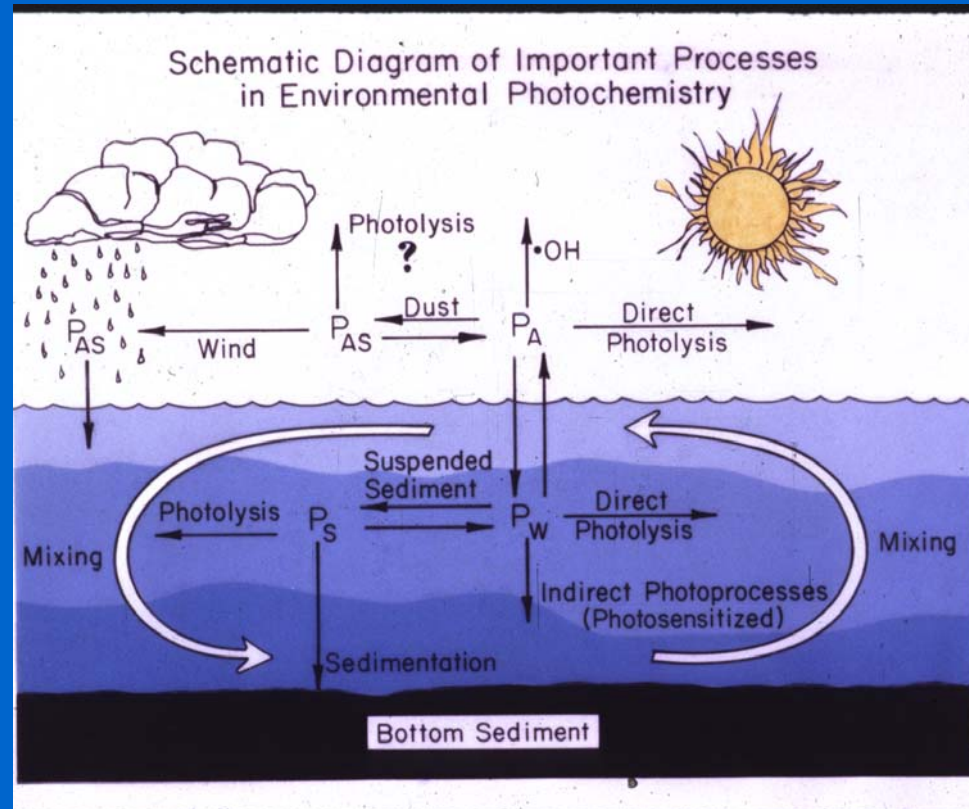
Aquatic Exposure Processes

- Loadings (rain, secondary drift)

- Water-Borne Transport
  - linkage to hydrodynamic models

- Sediment Transport
  - settling/resuspension, bbl exchange (3MRA/TRACE)

- Chemical Speciation
  - sorption kinetics; multi-phase (sand/silt/clay; labile and refractory) models

- Transformation and Transport Losses
  - physical (burial), chemical (photolysis), biolysis

Bioaccumulation and Aquatic System Simulator (BASS) -- Craig Barber
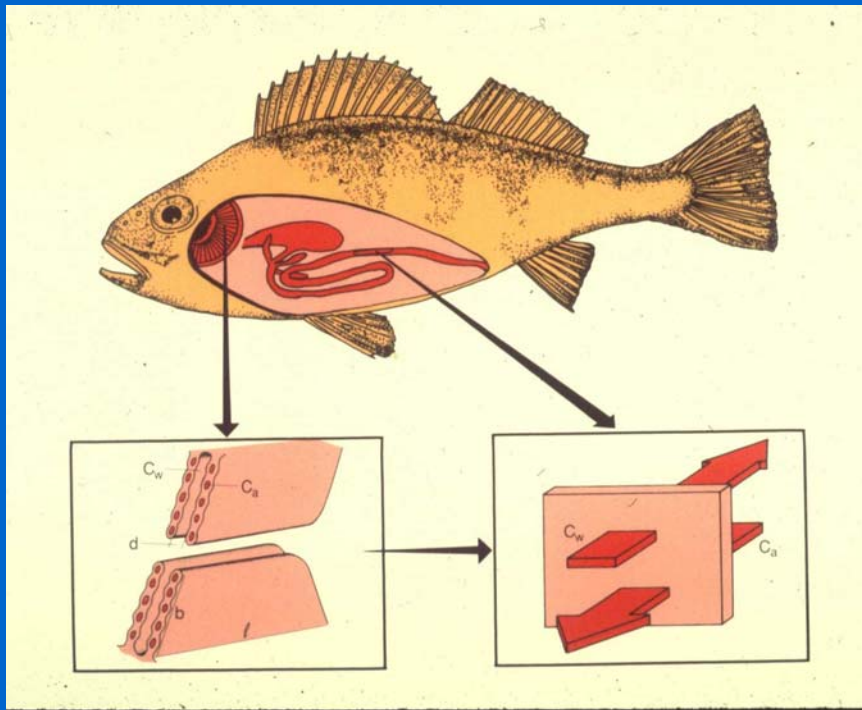
- Growth, population and bioaccumulation dynamics of multi-species, age-structured fish communities
- Ecological effects
  - additive lethality
  - growth depression
  - temperature

BASS Objectives

- Graphical User Interface (GUI)

- Scenario Building

  - Species databases: physiology, ecology, morphology

  - Canonical communities: species composition, food web structure, standing stocks

BASS Objectives

- Coupled (internal) dynamic models for non-fish components of aquatic ecosystems
  - benthos
  - phytoplankton (lakes and reservoirs)
  - periphyton (streams and wetlands)
  - zooplankton

Exposure Modeling   Summary

- Spray drift (estimation of off-target deposition)
- Crop interception and degradation/washoff on canopy
- Soil interception, pesticide degradation and sorption in soil
- Simulation of runoff, erosion and pesticide transport
- Simulation of subsurface drainage (e.g., tile drains) and consequent pesticide transport to streams and ponds
- Simulation of receiving water bodies: pesticide loading, physical dispersion, chemical and biological degradation, partitioning between limnetic and benthic subsystems
- Contamination of human and wildlife food chains

National Datasets

- Scale: MLRA/State
- When available: 1997 National Resource Inventory (NRI)
  - crop/soil association
- SAMSON: Solar and Meteorological Surface Observation Network (239 stations with 35 years of data)


SAMSON Stations and State Parts of MLRA
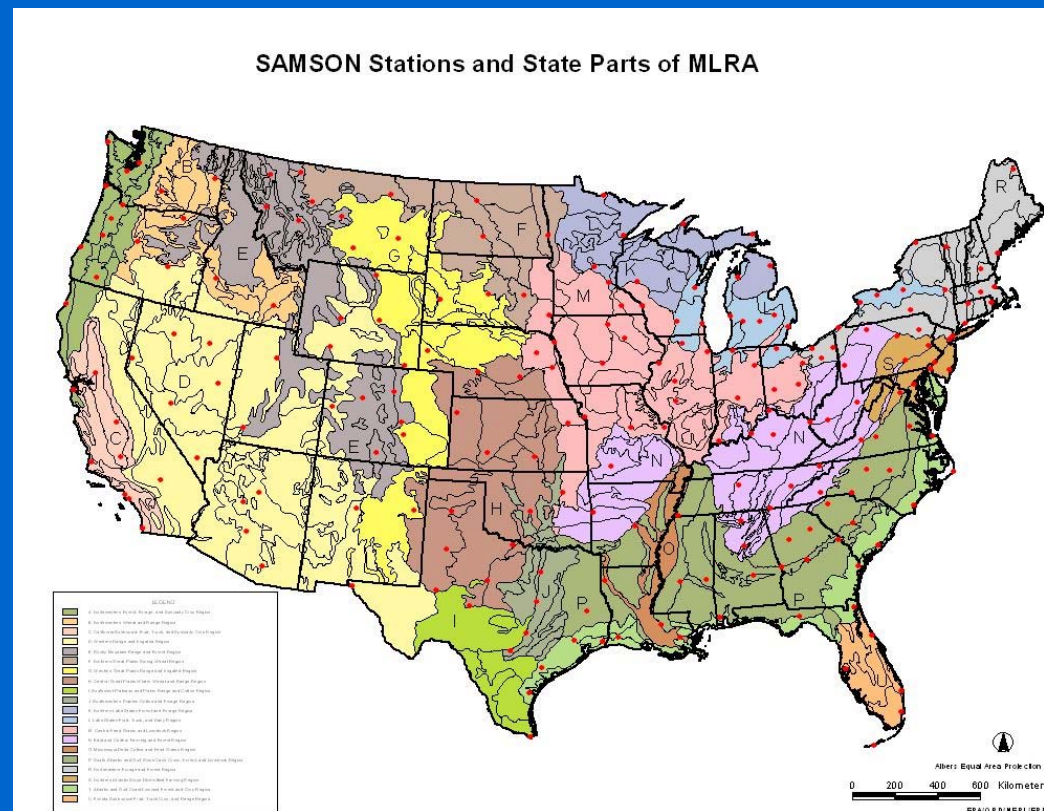
ECOFRAM Risk Metrics

- Interpreting time series for effects analysis
- Acute and chronic events, long-term exposures, other toxicological "events"
- Mortality
  - LC_{50} and "Levels of Concern"
    - (e.g., 2 µg/L NOAEL or LOAEL concern threshold)
  - Mortality response curves
- Presented at SETAC 1999/2000

Model Time Series Output
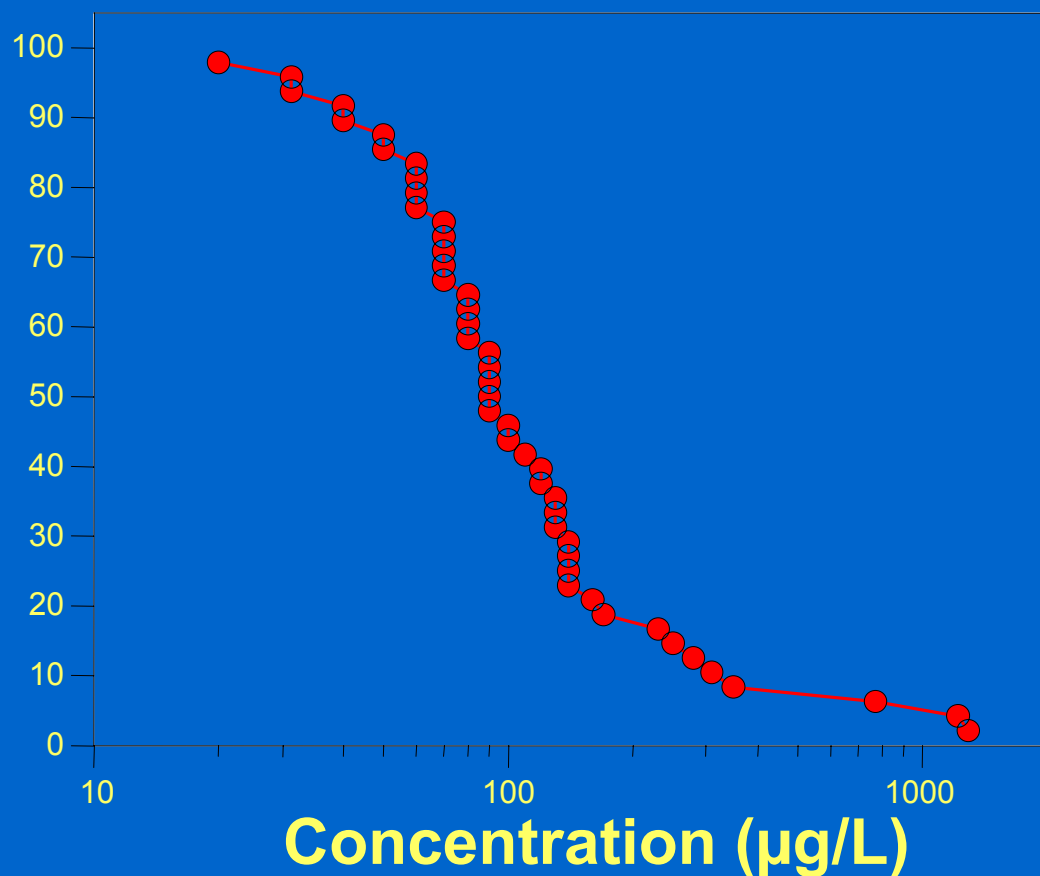
- For events > 2 μg/L:
- duration
- recovery
- magnitude
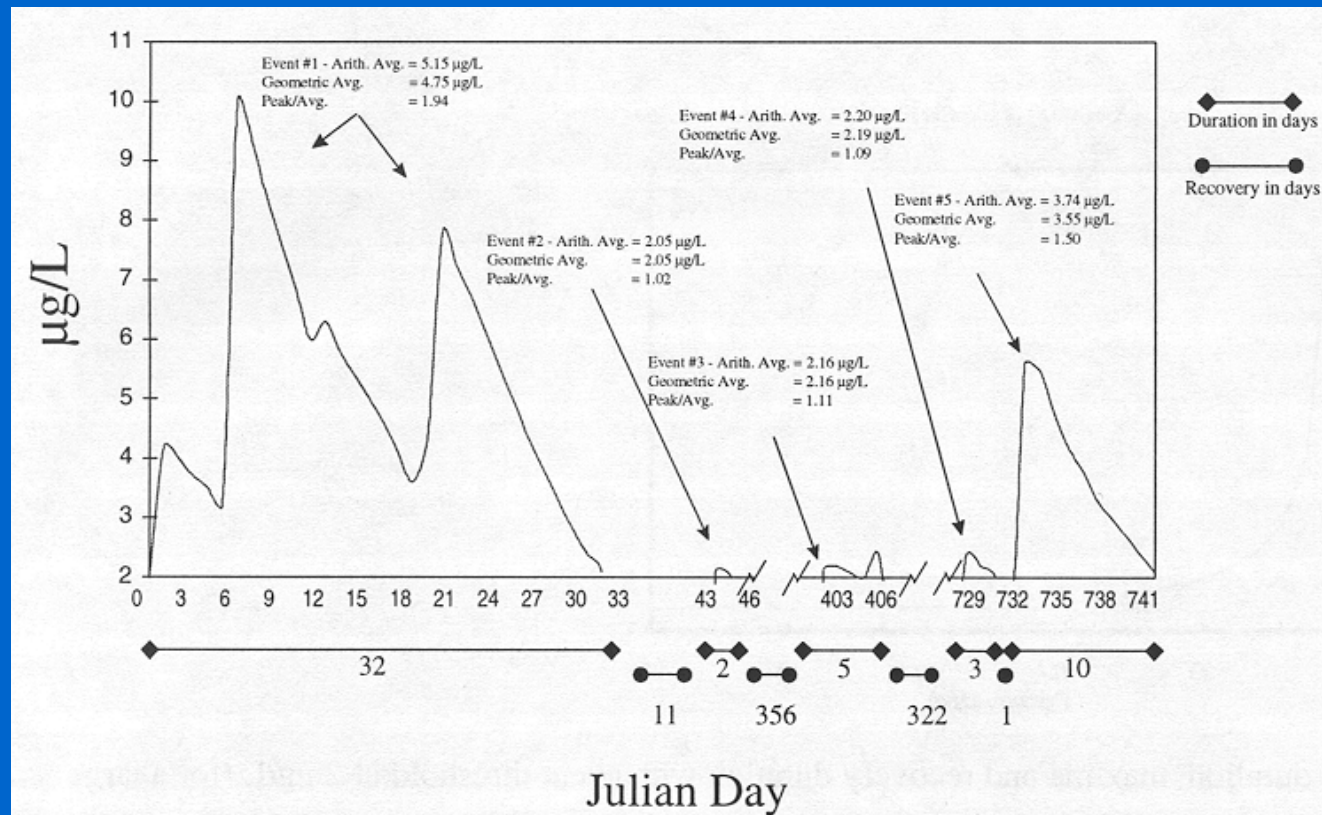
Exposure Distributions

- Annual Maximum 4-Day Series

- 95th %tile events in agricultural watersheds in Land Resource Region P

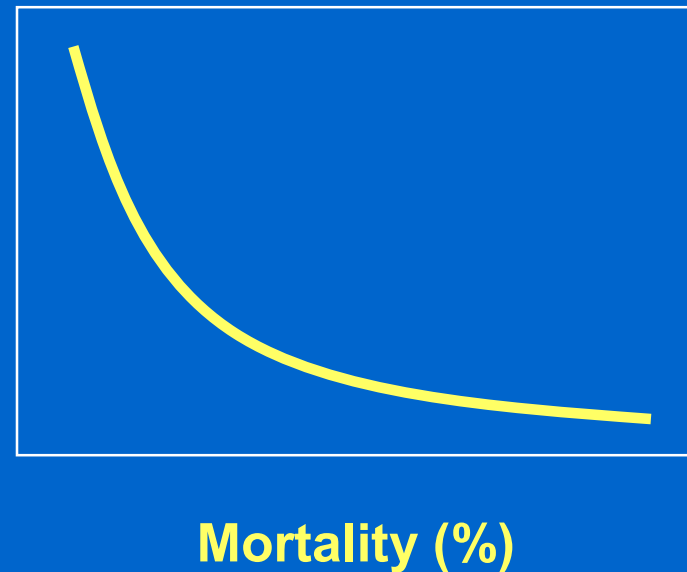- Cumulative distribution of maximum LOC exceedence across all MLRA

Effects Linkages and Risk Characterization:
Magnitude and Probability (ECOFRAM Implementation)

Organo-Phosphorus Insecticides
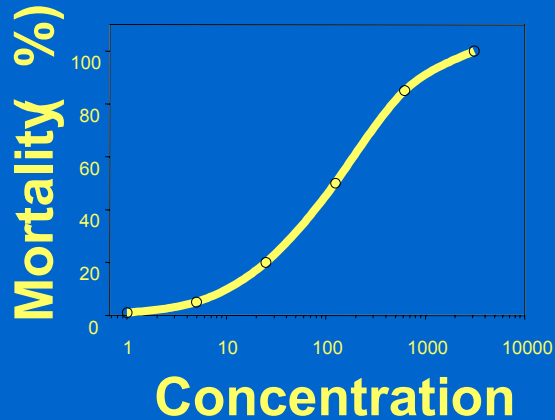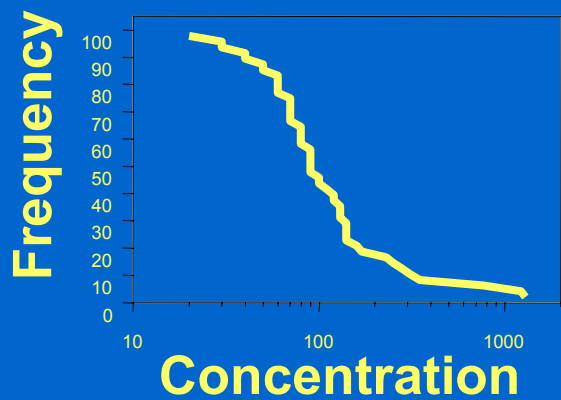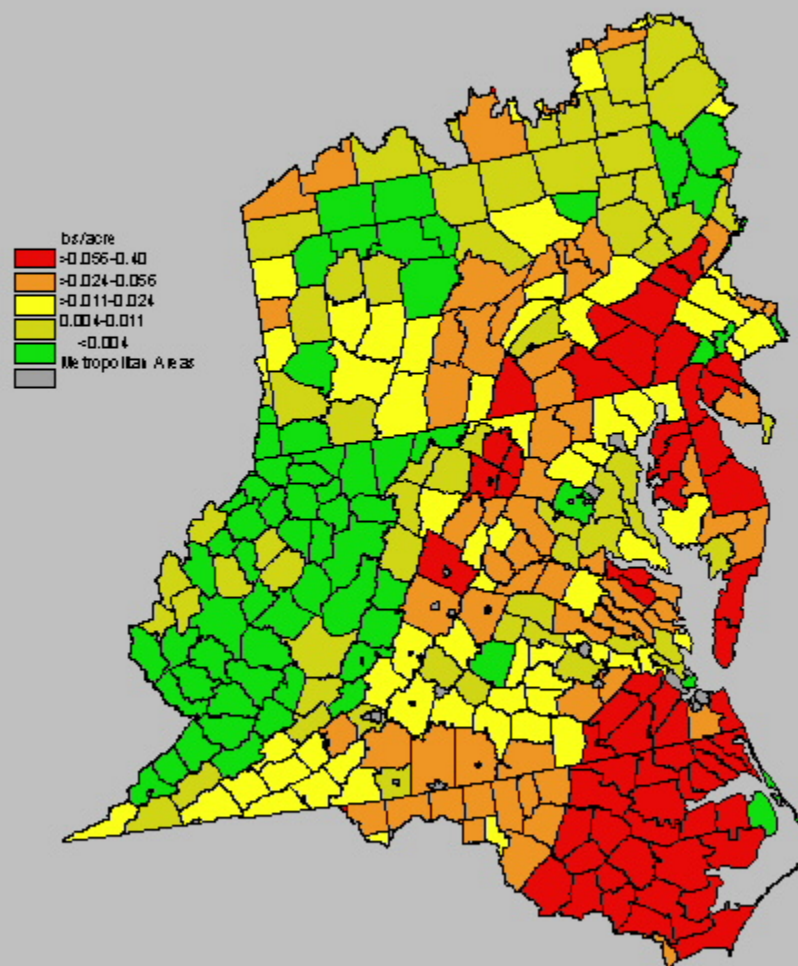
- Spatial distribution of
  - use patterns
  - acute events
  - ranking of long-term aquatic exposure concentrations

lbs/acre
>0.056-0.40
>0.024-0.056
>0.011-0.024
0.004-0.011
<0.004
Metropolitan Areas

Products and Outputs

- EXAMS User Manual (EPA/600/R-00/081)
- PRZM 3.12 Manual (responding to reviews)
  - (validation report at http://www.femvtf.com)
- BASS 2.1 Manual (in revision)
- AgDrift validation papers and Manual
- (06/2001) Review of validation studies
- (09/2001) APM 131: Tier 2 probability-based methodology report (ECOFRAM/OPP)

Questions, Comments...

USDA Agriculture Handbook 590